Evaluation of the Elastic Properties of Thin Films by Finite Element Method

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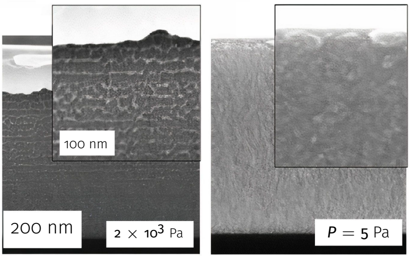


$Cu_{50}Zr_{50}$ amorphous thin films generated by pulsed laser deposition within a background gas of different pressure.

[1] Ghidelli et al. *Novel Class of Nanostructured Metallic Glass Films with Superior and Tunable Mechanical Properties.* In: Acta Materialia **203** (2021), page: 116955.

Applications (examples)

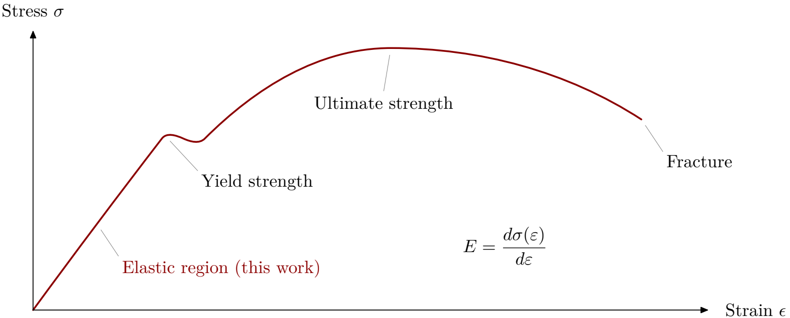
- Anti-corrosion properties.
- Change friction coefficients.
- Anti-reflection coating.
- Use for chemical sensors.
- Deposition of hard layers.
- Insulating/conducting films.
- Tune the bandgap of SC.

Deposition (examples)

- Magnetron sputtering.
- Vacuum thermal evaporation.
- Electroplating technique.
- Chemical vapor deposition

Objective : Predict the elastic properties of thin film coatings deposited on a substrate by FEM, with applications to Cu/Zr thin films deposited by magnetron sputtering.

- ✓ Elasticity : Elongation of interatomic bonds, reversible process.
- ✗ Plasticity : Breaking and reforming of interatomic bonds, irreversible process.



1 $\Rightarrow$ Description of the governing equations (Cauchy momentum equation).

2 $\Rightarrow$ Simulation of atomic flux during magnetron sputtering (Monte Carlo).
Estimation of the energy and angular distributions of the particles.

3 $\Rightarrow$ Simulation of the thin film growth on the substrate (Monte Carlo).

4 $\Rightarrow$ Meshing and boundary conditions (including applied stress on the film).
Estimation of the elastic properties with the numerical results.
Comparison of those properties (Young's modulus) with the literature.

Discrete

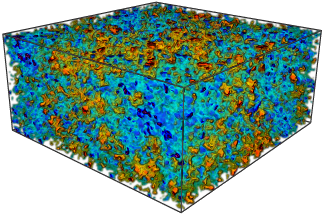
Discrete / Continuum

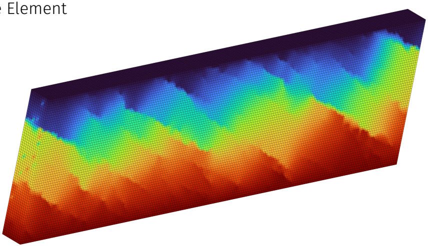
Continuum

Molecular Dynamics

Atomistic Finite Element
Discrete Finite Element

Finite Element Method





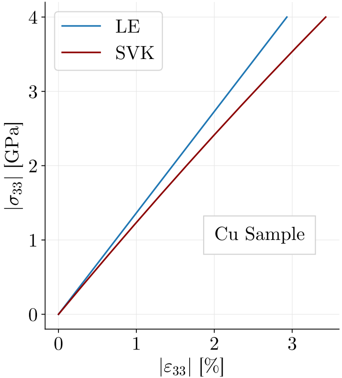
High computational costs

Lower computational costs

Equation to Solve

Cauchy momentum equation : $\nabla \cdot \sigma\left[\varepsilon(\mathbf{u})\right] + \cancel{\rho \mathbf{g}} = \cancel{\rho \frac{\partial^2 u}{\partial t^2}} \quad \text{in} \;\; \Omega(\mathbf{u})$

Stress-Strain Curve $\Rightarrow E$



Two Models

Linear SST/SET (LE)

$$\nabla_S \cdot \sigma_S = 0 \;\; \text{on} \;\; \Gamma_S$$

$$\varepsilon = \frac{1}{2}\left(\nabla u + \nabla u^\top\right) \;\; \text{in} \;\; \Omega$$

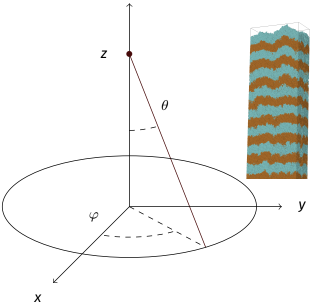
Non-Linear SVK

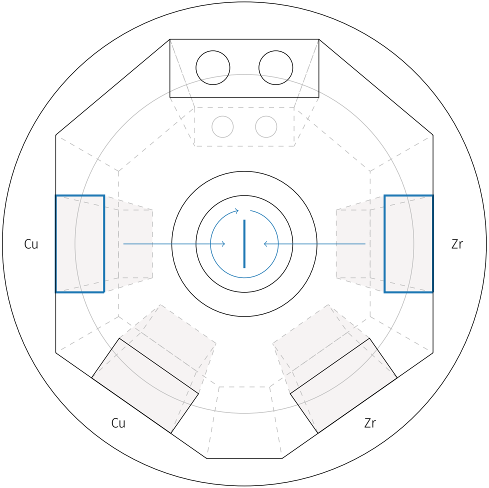
$$\varepsilon = \frac{1}{2}\left(\nabla u + \nabla u^\top + \nabla u \nabla u^\top\right) \;\; \text{in} \;\; \Omega(\mathbf{u})$$

Deposition and Results

- **Step 2** : Simulation of magnetron sputtering.
- **Step 3** : Thin film growth on the substrate.
- **Step 4** : Application of FEM and comparison.

- **Transport in Gaz Phase by MC Simulation.**



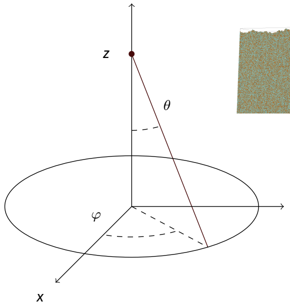


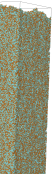
Single cathode mode

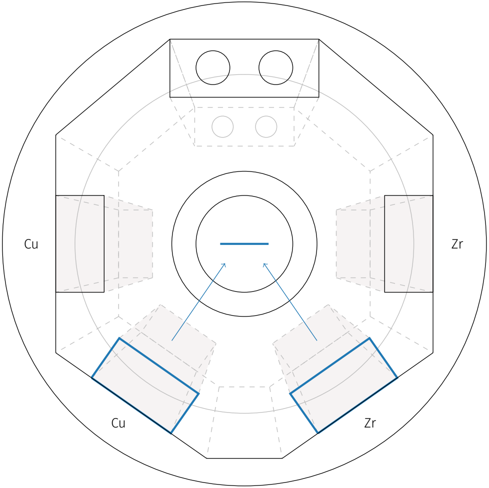
$\rho_{\mathrm{E}}(E, p) =$ Energy distribution.

$\rho_{\mathrm{A}}(\theta, p) =$ Angular distribution.

- **Transport in Gaz Phase by MC Simulation.**







Double cathode mode

$\rho_E(E, p)$ = Energy distribution.

$\rho_A(\theta, p)$ = Angular distribution.

$\rho_E \longrightarrow$

$\rho_A \longrightarrow$

NASCAM (KMC)

Output $\longrightarrow$

Kinematic Monte Carlo

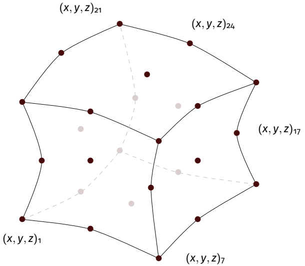
The film growth on the substrate is simulated by NASCAM (LARN development).

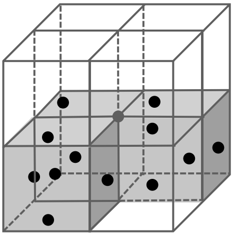
The finite element mesh and the boundary conditions (including applied stress) are generated according to those results.

One can finally compute the overall elastic response of the thin film.

Discretization of the Film

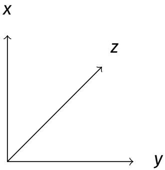
- Solid finite element if its filling fraction is $f \geq f_M$. Empty element if $f < f_M$.
- Single chemical species (Cu or Zr) or molecule (CuZr) per finite element.
- Enforce a flat surface where the load is applied, periodic BC in the (x, y) plane.





Global coordinates

$\Omega \in \mathbb{R}^3$

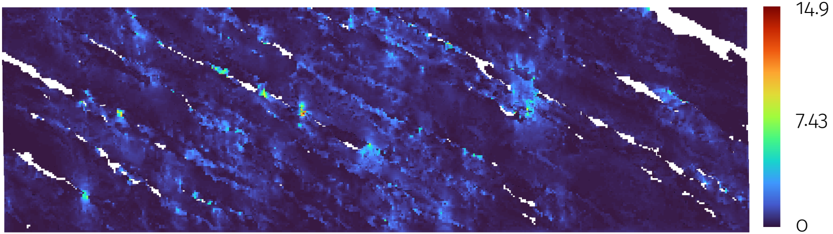


Additionnal Parameters

- Take a numerical model (SST/SET - SVK).
- Choose a finite element order.
- Properties of the atoms and substrate.
- Apply the stress on the film (mesh).
- Compute elastic response.

$$\begin{cases} \text{Model} = \text{SVK} \\ \text{Lattice constant} = 0.34 \text{ nm} \\ \text{Element size} = 1 \times 1 \times 1 \text{ Lc}^3 \\ E = 130 \text{ GPa } \nu = 0.34 \\ \text{Applied stress : } -0.1 \text{ GPa} \\ \text{periodic BC} \end{cases}$$

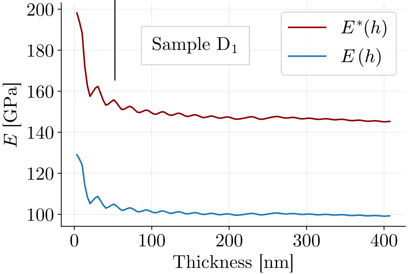
$\sigma_{\text{VM}}(\mathbf{x})$ for a pure Cu film (in GPa)



40×11 nm layers

Discontinuities due to the layers

With stiff substrate



Film only

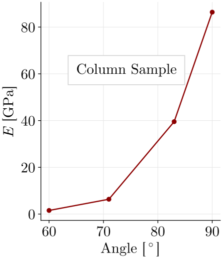
Young's Modulus

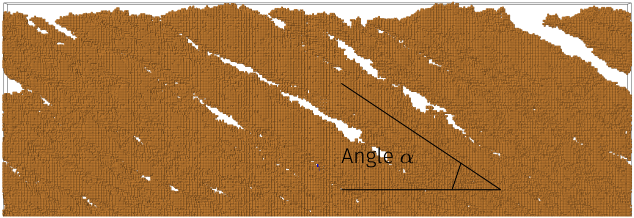
Number of layers

In addition to the displacement field, the stress field computed by finite element can be used to estimate **when** and **where** plastic deformations will occur.

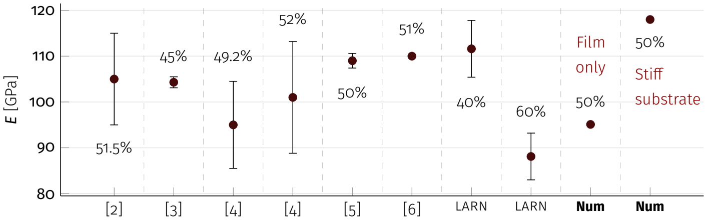
Influence of the Columnar Structure

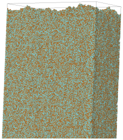
- Columns may be generated by orienting the substrate with respect to the target.
- The angle (with respect to the horizontal) of the columns highly influences the overall elastic response of the film.
- The stiffness of the substrate has a low influence on the vertical Young's modulus when the film displays a columnar structure.

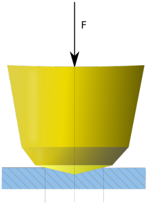




Experimental results by Nanoindentation (CuZr) | Numerical







[2] P. Coddet et al. *On the Elastic Modulus and Hardness of Co-Sputtered Zr-Cu-(N) Thin Metal Glass Films.* In: Surface and Coatings Technology **206** (2012), page: 3567–3571.

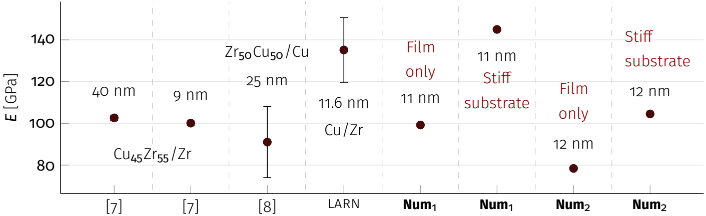
[3] M. Abboud. *Micromechanical Characterization of Metallic Glass - Crystalline Nanocomposite Coatings.* Master thesis: Middle East Technical University (2018), Turkey.

[4] M. Apreutesei et al. *Microstructural, Thermal and Mechanical Behavior of Co-Sputtered Binary. Zr-Cu Thin Film Metallic Glasses.* In: Thin Solid Films **561** (2014), page: 53–59.

[5] A. Rauf et al. *Binary Cu-Zr Thin Film Metallic Glasses with Tunable Nanoscale Structures and Properties.* In: Journal of Non-Crystalline Solids **408** (2018), page: 95–102.

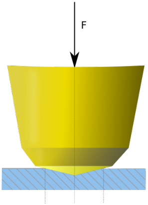
[6] P. Zeman et al. *Amorphous Zr-Cu Thin-Film Alloys with Metallic Glass Behavior.* In: Journal of Alloys and Compounds **696** (2017), page: 1298–1306.

Experimental (Nanoindentation) | **Numerical Simulations (Cu/Zr)**



20% of porosity

30% of porosity



[7] M. Abboud. *Micromechanical Characterization of Metallic Glass - Crystalline Nanocomposite Coatings*. Master thesis: Middle East Technical University (2018), Turkey.

[8] H.J. Pei et al. *Tension Behavior of Metallic Glass Coating on Cu Foil*. In: Materials Science and Engineering A **528** (2011), page: 7317–7322.

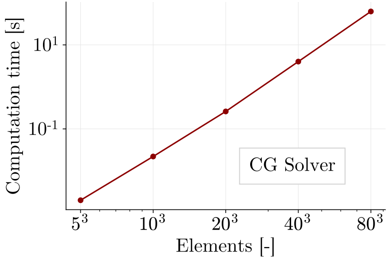
Summary

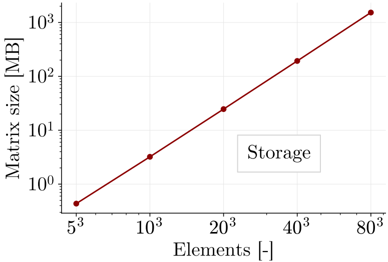
- Comparison between linear SST/SET, LE and non-linear SVK models.
- Good agreement with experimental data, but E is sometimes underestimated.
- Study of the influence of the nanostructure on the elastic response.
- Study of the influence of the porosity on the elastic response.
- Difference between experimental and numerical conditions.

Perspectives

- **Numerical efficiency** : GPU acceleration, memory optimization, multithreading.
- **Physics** : Better mesh, contact mechanics or different material model.
- **General** : Influence of homogenization within the elements.
- **General** : Complete analysis of the CuZr structure.

Bottleneck performances for a plain cubic block of linear finite elements with periodic boundary conditions and a stress applied to the top surface.
The FEM model is the linear elasticity.





Compiler : C++ 14 gcc with -O3 optimisation
Processor : x64 Intel(R) Core(TM) i7-7700HQ CPU @ 2.81 GHz 16 GB RAM.

NASCAM Integration